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A Framework for Interpolating Scattered Data using Space-filling Curves

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Abstract. The analysis of spatial data occurs in many disciplines and covers a wide variety activities. Available techniques for such analysis include spatial interpolation which is useful for tasks such as visualization and imputation. This paper proposes a novel approach to interpolation using space-filling curves. Two simple interpolation methods are described and their ability to interpolate is compared to several interpolation techniques including natural neighbour interpolation. The proposed approach requires a Monte-Carlo step that requires a large number of iterations. However experiments demonstrate that the number of iterations will not change appreciably with larger datasets.

1 Introduction

Spatial interpolation is one of the many tools available for spatial data mining [10]. It is particularly useful in spatial analysis since it is often the case that data cannot be collected at every desired location due to practical issues such as cost. In addition the data may have missing values [11], that may require imputation. The literature for spatial interpolation is large and the interested reader is referred to [8] for an overview of available approaches in the practical context of environmental sciences.

Space-filling curves have been successfully used in a broad range of computational problems, for example in calculating efficiently all nearest neighbours [4] and image segmentation [9], see [1] for a comprehensive review. The primary reason for this is the fact that space-filling curves can be used to map multi-dimensional Euclidean data onto one dimension which partially preserves local spatial correlations, i.e. points that are close in the multidimensional space are likely to be close in the one dimensional ordering of the data.

[16] investigated the orderings of data along space-filling curves where the data has been repeatedly transformed using shape preserving transformations only. It was shown that the probability of an ordering is dependent on the spatial locations of the data in the higher dimensional space. This property was then used to construct novel shape descriptors for shape matching. The concern of this paper is to use the approach detailed in [16] for spatial interpolation. The essential idea is to transform the data-sites and query points using a shape preserving transformation and then map them onto a space-filling curve, where

a simple interpolation scheme is used to impute the value at each query point. This process is repeated using different shape preserving transformations and the resulting interpolations are then aggregated. The main motivation for this work is to produce a conceptually simple approach for interpolation in two or higher dimension that is also numerically robust and simple to implement.

In the next section, relevant methods for interpolating scattered data are discussed. After which space-filling curves are introduced with a brief overview of the construction of the Hilbert curve. Following this, the framework for performing spatial interpolation using space-filling curves is introduced. Experiments to demonstrate the utility of the approach are provided. The final section concludes with ideas for future research.

2 Scattered data interpolation methods

In the following discussion it will be assumed that there are n data-sites x_1, \dots, x_n with respective locations $\mathbf{x}_1 \dots \mathbf{x}_n$ and each data-site has a value denoted $z_1 \dots z_n$. In addition there are m query sites, $q_1 \dots q_m$ with location $\mathbf{q}_1 \dots \mathbf{q}_m$. It is at these locations that an imputed value is desired, i.e. we wish to estimate $\hat{f}(\mathbf{q}_j)$, for query site q_j .

There are a large array of methods available for spatial interpolation. The focus in this section will be on three methods for spatial interpolation. They have been chosen specifically because they are the higher dimensional analogues of the interpolation we do in one dimension and hence provide a clear comparison. They are *piecewise constant*, *piecewise linear* and *natural neighbour* interpolation.

Piecewise constant interpolation is a very simple approach to scattered data interpolation. The interpolated value, $\hat{f}(\mathbf{q}_j)$, for query site q_j is the value associated with the closest (in the Euclidean sense) data-site.

Piecewise linear interpolation for scattered data uses the Delauney triangulation, see e.g. [12], induced from the data-sites. The vertices in this triangulation are the data-sites. In, for example 2D, a query point will reside in one triangle. Let us assume that the vertices are the data-sites with indices p_{1j}, p_{2j}, p_{3j} , then

$$\hat{f}(\mathbf{q}_j) = \frac{\sum_{i=1}^3 a_{p_i} z_{p_{ij}}}{\sum_{i=1}^3 a_{p_i}},$$

where a_{p_i} is the Euclidean distance between the query point q_j and the vertex location $\mathbf{x}_{p_{ij}}$

Natural neighbour interpolation is a well known approach to interpolating scattered data, see for example [3]. This interpolation scheme involves calculating a weighted sum of data-site values that are natural neighbours (definition to follow) to the query point. There exist several approaches to calculating these weights, the most well known is *Sibson* interpolation and is calculated as follows. First the Voronoi tessellation is induced from the data-site locations. This consists of partitioning the region of interest into non-overlapping tiles. Each tile contains only one data-site and contains all locations that are closest to this data-site, Fig. 1(a).

The location of the query point is added to the list of data-sites and a new Voronoi diagram is produced. This is shown in Fig. 1(b) where the query point in this figure is denoted with a cross. This query point has its own Voronoi tile that contains regions taken from the original Voronoi tiles shown in Fig. 1(a). Data-sites that have had their Voronoi tile changed by the inclusion of the query point are called its natural neighbours. For a particular query point q_j

$$\hat{f}(\mathbf{q}_j) = \frac{\sum_i w_{ij} z_i}{\sum_i w_{ij}},$$

where w_{ij} is the area from the query point tile that was originally part of the Voronoi tile for the i th data-site.

Conceptually natural neighbour interpolation is relatively straightforward however computing it efficiently is rather involved [7]. Indeed approximations that rely on discretising the region of interest have been proposed to produce more efficient algorithm [13]. Natural neighbour interpolation is defined for two or more dimensions, since in 1D, the procedure for natural neighbour interpolation reduces to piecewise linear interpolation. Briefly, in 1D the Voronoi tiles are simply intervals and the natural neighbours of a query point are its predecessor and successor data-sites. Since we shall be using linear interpolation in 1D in our proposed approach, we consider natural neighbour interpolation to be a relevant method to compare against.

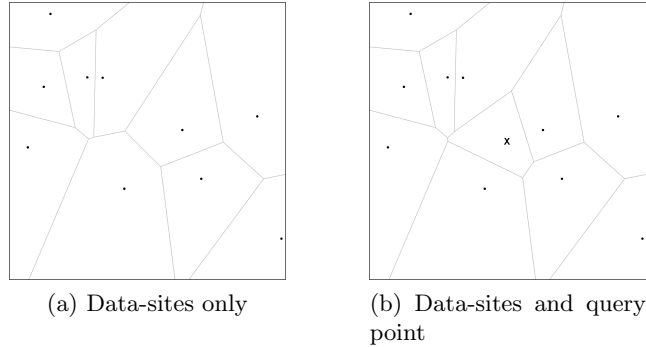


Fig. 1: Voronoi diagrams used for natural neighbour interpolation weight calculation. The query point q_j is denoted by a cross located in the centre of (b).

3 Space-filling curves

A space-filling curve is typically defined as a continuous mapping from the unit interval $[0, 1]$, onto d -dimensional Euclidean space where the image consists of all points within the compact region $[0, 1]^d$.

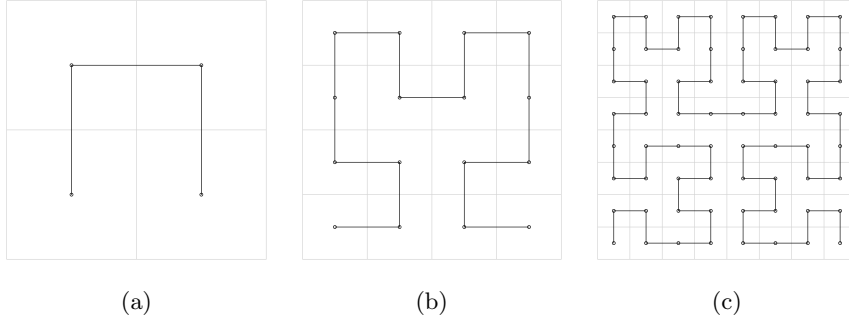


Fig. 2: First three iterations for Hilbert curve construction, the circles denote the centres of the sub-squares.

Fig. 2 shows the construction of the Hilbert space-filling curve. A square is sub-divided into four sub-squares which are given a specific order and orientation. Joining the centres of these sub-squares by following their order produces a polygon approximation to the Hilbert curve, Fig. 2(a). These sub-squares are themselves recursively subdivided. Figs 2(b,c) show the polygon curve for second and third iteration respectively. In the limit as the number of iterations tends to infinity, the polygon curve tends to the Hilbert curve.

A detailed explanation regarding space-filling curves and their construction can be found in [1], [14]. The code used in the paper is based on [15].

4 Framework for Interpolation

There are three stages in the proposed framework for interpolation, denoted *shape preserving embedding*, *one-dimensional interpolation* and *aggregation*. Each stage is described separately in the following sections.

4.1 Shape Preserving Embedding

The first stage involves ordering the data-sites (and query locations) in multidimensional space along a space-filling curve. The entire process is demonstrated graphically for the 2D case in Fig. 3. For simplicity it is assumed that interpolation is required over a square region of interest containing all the data-sites, Fig. 3(a). A shape preserving transformation is applied that maps the region of interest onto the unit square denoted by the grey region in Fig. 3(b). Each data-site (and query point) can then be ordered along a Hilbert curve. Fig. 3(c) shows each data-site joined to their predecessor and successor along the space-filling curve.

Let e denote a shape preserving transformation that embeds the query points and data-sites successfully into the unit square. The transformation is in fact a

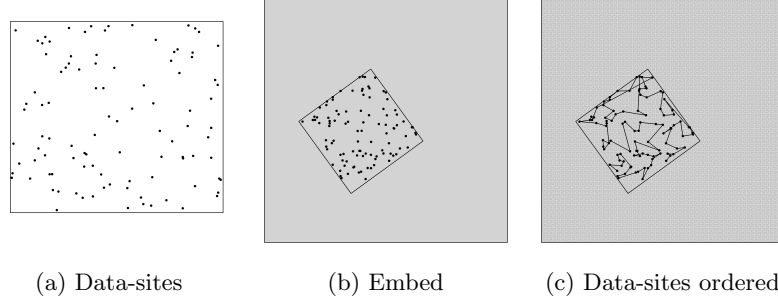


Fig. 3: Embedding data-sites onto Hilbert Curve.

composite, comprising a translation, a rotation, a reflection (with probability 0.5) and a scaling. Details of the embedding can be found in [16], the maximum scale factor in this study is 10. For reasons of computational simplicity the region of interest, i.e. domain over which the interpolation function $\hat{f}(\cdot)$ is to be estimated is assumed to be a discretised square with resolution 2000×2000 .

Let h denote a function that maps a point in the unit square onto the unit interval using a Hilbert curve. The Hilbert index, t_i , for the i th data-site is

$$t_i = h(e(\mathbf{x}_i))$$

and similarly for query sites. The data is then sorted in ascending Hilbert index order. Let this ordering function be denoted by π , then $t_{\pi(d_i)}$ and $t_{\pi(q_j)}$ are both non-decreasing for $i = 1, \dots, n$ and $j = 1, \dots, m$ respectively.

4.2 One-Dimensional Interpolation

Once a Hilbert index has been associated with each datum, interpolation can proceed using any 1D interpolation method. For this study 1D piecewise constant and 1D piecewise linear interpolation (described in Section 2), denoted *Hilbert-Const* and *Hilbert-Linear* respectively are used. Both these methods are trivially simple to implement and due to their simplicity they are amenable to further analysis which can be achieved without the need of a ground truth function to interpolate, see Section 6.

4.3 Aggregation

Let g denote a function that encapsulates the two stages described above, such that interpolated value for the query site q_j is

$$\hat{f}(\mathbf{q}_j) = g(\mathbf{q}_j, \mathbf{x}_{1\dots m}, z_{1\dots m}, h, Q_1, e).$$

Where Q_1 denotes a plug-in one-dimensional interpolation function and e a shape preserving transformation. Recalling that $\mathbf{x}_{1\dots m}, z_{1\dots m}$ are the data-site locations

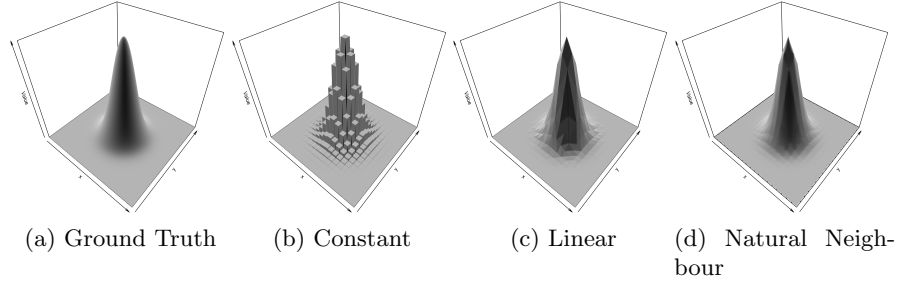


Fig. 4: Bivariate Gaussian test function and interpolated functions using standard 2D approaches based on data-sites located on a regular 21×21 grid.

and data-site values respectively; h is the Hilbert mapping, note that this can be replaced with other space-filling curve mappings.

Let e_1, \dots, e_η be identically and independently drawn legitimate transformations, further details for the sampling regime can be found in [16]. The aggregated interpolated value for the query site q_j is simply the average interpolated value, i.e.

$$\hat{f}(\mathbf{q}_j) = \frac{1}{\eta} \sum_{k=1}^{\eta} g(\mathbf{q}_j, \mathbf{x}_{1\dots m}, z_{1\dots m}, h, Q_1, e_k).$$

5 Experiments

The following experimental design has been motivated by [6]. The interpolation schemes are tested by evaluating the mean squared error (MSE) and the maximum absolute error (Max Error) between interpolated values and a ground truth function. For the ground truth Franke’s function [6] has been selected, see Fig. 6(a).

It is also instructive to visualise the interpolation, for this task a bivariate Gaussian is used see Fig. 4(a). The experiments are organised as follows. First the focus is on visualising the resulting interpolations, then a more formal approach to evaluating the interpolation methods is performed. Henceforth piecewise linear and piecewise constant shall be referred to as linear and constant respectively.

5.1 Visualising the Interpolated Function

This experiment uses data-sites located on a 21×21 regular grid spanning the entire region of interest. It should be noted that for the special case of data-sites located on regular grids there exist specific interpolation schemes that should do better than the general scattered data interpolation approaches shown here. However a regular grid generates easily interpretable images. Fig. 4 shows the resulting interpolation when using the spatial interpolation techniques described in Section 2.

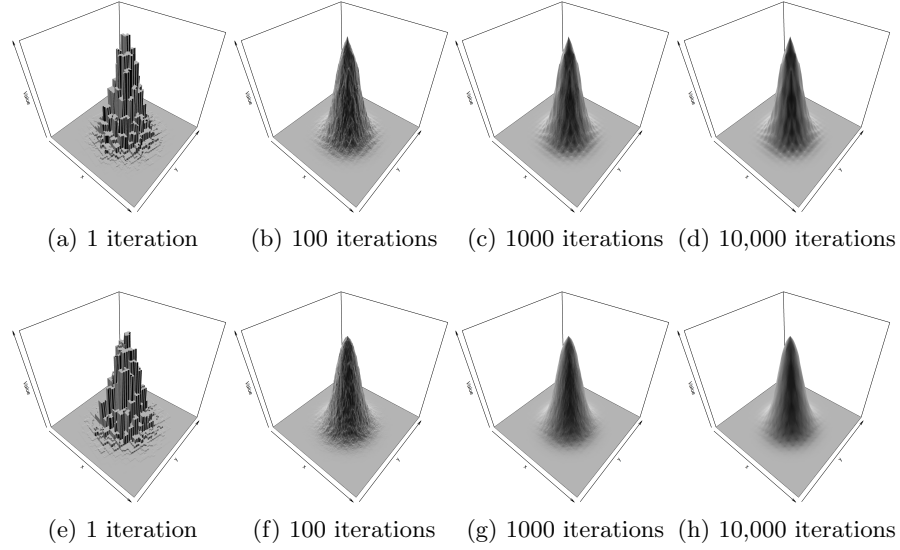


Fig. 5: Hilbert-Const Interpolation of a Bivariate Gaussian based on data-sites located on a regular 21×21 grid. Top row Hilbert-Const Interpolation, bottom row Hilbert-Linear Interpolation.

It is clear that constant interpolation, Fig. 4(b), does a poor job of reconstructing the ground truth. Linear interpolation, Fig. 4(c) does much better but with strong visible linear artifacts. Finally in Fig. 4(d) natural neighbour interpolation is much smoother. Although artifacts arising from the data-site locations are visible.

Fig. 5(a-d) shows the interpolated function using Hilbert-Const with increasing number of iterations. Fig. 5(a) shows the interpolated function after one iteration is similar to constant interpolation shown in Fig. 4(b). As the number of iterations increases, the interpolated function becomes less noisy and at 10,000 iterations the function is visibly similar to natural neighbour interpolation but with more pronounced bumps.

Fig. 5(e-h) shows the interpolated function Hilbert-Linear. The first iteration may look similar Hilbert-Const however closer inspection should reveal that there are no flat regions on the tall peaks. At 10,000 iterations the interpolated function appears smoother than both natural neighbour and Hilbert-Const. In contrast to both natural neighbour and Hilbert-Const an artifact due to the data-site locations manifests itself as small dimples.

Franke's bivariate function, shown in Fig. 6(a), is a more challenging surface to interpolate. Fig. 6 also shows the interpolated functions using the interpolation methods described in Section 2 and the resulting interpolated function after the first and 10,000th iteration for both Hilbert-Const and Hilbert-Linear. Visually these results are consistent with those of the bivariate Gaussian.

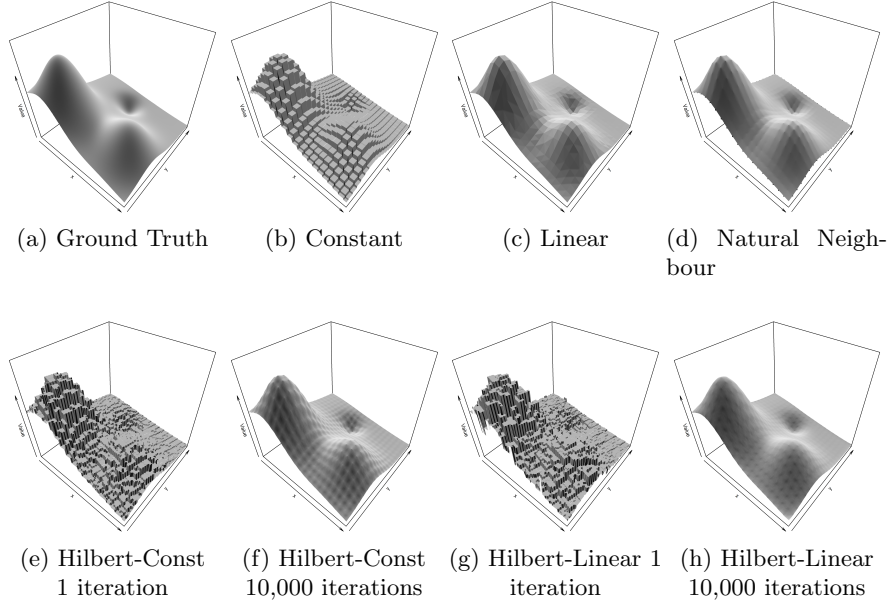


Fig. 6: Franke’s bivariate test function and interpolated functions using standard 2D approaches based on data-sites located on a regular 21×21 grid.

5.2 Scattered Data Interpolation

The following experiments focus on more quantitative measures of the quality of an interpolation. Scattered data-sites are generated by selecting uniformly at random a location on a 2000×2000 grid without replacement, this is to ensure that all the data-site locations are unique. The number of data-sites used in the experiments are 100, 300 and 500. Finally, for completeness, the data-sites using regular locations used in the first experiment will also be used (which has 441 data-sites). The number of aggregation iterations η is set to 50,000. Natural neighbour interpolation is not defined outside the convex hull of data-sites, so to make all the results commensurate only query sites within the convex hull are included in the analysis.

Table 1 shows the evaluations for the three standard interpolation methods (natural neighbor interpolation is denoted NN in this table) and the two proposed approaches for different sets of data-site locations and number. Notable observations include the following. Constant Interpolation in 2D is consistently poor; Linear interpolation in 2D in most cases performs better than natural neighbour.

Hilbert-Const has lower Max Error than natural neighbour for all scattered data sets, but natural neighbour performs consistently better with respect to

Table 1: Performance of interpolation schemes with respect to Maximum Absolute Error and for Mean Squared Error for the Franke Function.

# Data-sites	100		300		500		441 Regular	
	Max Err	MSE	Max Err	MSE	Max Err	MSE	Max Err	MSE
Constant 2D	0.421	0.00463	0.219	0.00147	0.173	0.000821	0.119	0.000529
Linear 2D	0.229	0.00181	0.139	0.000313	0.109	8.04e-05	0.0185	1.24e-05
NN 2D	0.249	0.00202	0.147	0.000332	0.0965	7.9e-05	0.0188	1.2e-05
Hilbert-Const	0.234	0.00239	0.117	0.000407	0.0635	0.000151	0.0217	2.03e-05
Hilbert-Linear	0.308	0.00381	0.0975	0.000516	0.0704	0.000135	0.0279	4.85e-05

MSE. The performance difference between Hilbert-Linear and Hilbert-Const is somewhat inconclusive but it appears that Hilbert-Const performs better.

A key issue with the proposed approach is the number of aggregation iterations required to produce a reasonable interpolation. Fig. 7 shows the number of aggregation iterations against MSE and Max Error for the Hilbert-Const interpolation of Franke’s function. The convergence is largely independent of the number of data-sites and there is little to gain after around 1000 iterations. A similar result has been obtained for Hilbert-Linear interpolation.

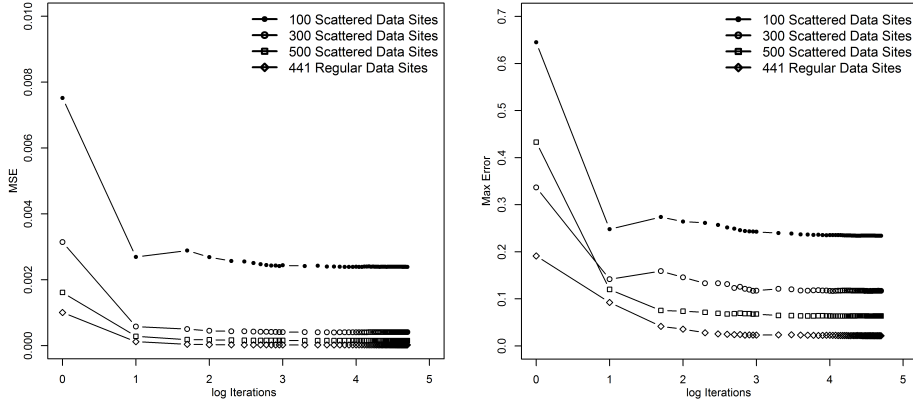


Fig. 7: Number of aggregation iterations versus MSE (leftmost graph) and Max Error (rightmost graph). Note the x-axis has a base-10 log scale.

In this section, analysis of interpolating specific functions was considered. In the next section the proposed approach is re-interpreted so that we can reason about it by considering only the location of the data-sites, i.e without the need of a ground truth function to interpolate.

6 Further Analysis

Hilbert-Const interpolation has a particularly simple interpretation. It can be viewed as a simple weighted sum of data-site values. The weight denoted p_i is

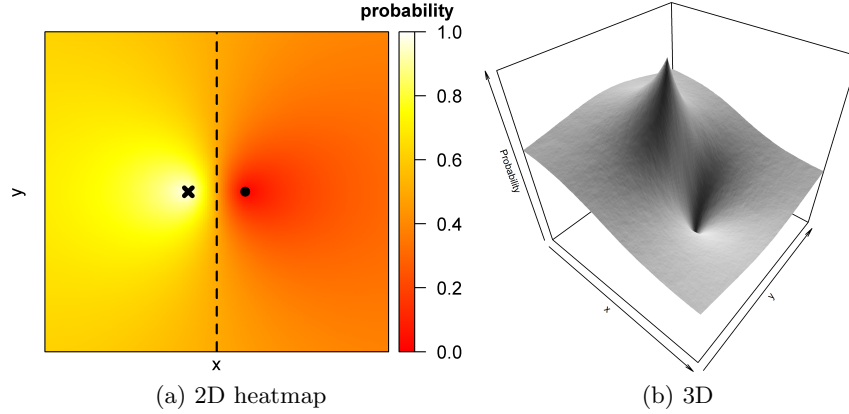


Fig. 8: Probability mass function showing the probability that the nearest neighbour is the data-site denoted by an \times .

the probability that data-site x_i is the nearest neighbour to q_j along the Hilbert curve under the Monte Carlo sampling described in the Aggregation Section, i.e.

$$\hat{f}(\mathbf{q}_j) = \sum_i^n p_i z_i \quad (1)$$

Consider the case where there are only two data-sites, denoted \times and \bullet , located within a region of interest shown in Fig. 8(a) (ignoring the heatmap for the moment). Under Euclidean distance, locations that are closest to the data-site denoted by an \times are to the left of the dashed line.

The heatmap represents all the possible query site locations within the region of interest and shows the probability the \times data-site is the nearest neighbour under the Monte Carlo sampling, with $\eta = 50,000$. Fig. 8(b) shows the same probability mass function but in 3D. It is clear that there is a discontinuity at the peak (corresponding to the \times data-site).

Referring back to Equation 1, for the interpolated function $\hat{f}(\cdot)$ to be continuous, both p_i and z_i are required to be spatially continuous over the region of interest. Assuming that the function to be interpolated is indeed continuous, i.e. z_i is continuous, then p_i needs to be continuous. As has been noted, p_i is not continuous at data-sites. Hence the interpolated function will not be continuous at data-sites. Note that natural neighbour interpolation also has this issue. The smoothness of probability mass function elsewhere in Fig. 8(b) is consistent with p_i being continuous everywhere apart from at data-sites.

A final observation from the heatmap in Fig. 8(a) is the probability mass function behaves sensibly since in general the closer to data-site \times the higher the probability. Fig. 9 shows the average number of data-sites that contribute to a query location. For the scattered data it is clear the average number is largely

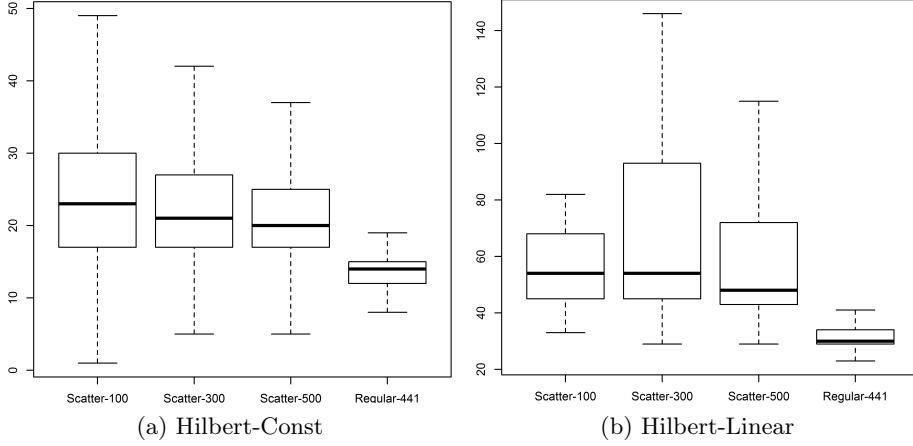


Fig. 9: Number of non zero weighted data-sites for each query location. Hilbert-Linear has more than Hilbert-Const since for linear interpolation uses two data-sites for interpolation whereas constant only requires one.

independent of the increasing number of data-sites. This is a crucial observation for the utility of the proposed approach for large datasets. It suggests that the interpolation is local to the query data-site.

There is one exception, query points near the boundary of the region of interest. Fig. 9 show there is a large variance in the number contributing data-sites per query site. This phenomena is due to the space-filling curve exiting region of interest and entering at some other location along the boundary. This behaviour is not necessarily wrong, it is making the assumption that the function is homogeneous around the boundary. One way to remove this edge effect is to introduce a post-processing step that keeps the closest w contributing data-sites for each query site near the boundary, where w is the overall mean.

7 Conclusion and Future Work

This paper proposed a novel framework to interpolating scattered data. The approach is conceptually easy to understand and straightforward to code and delivers results that are in some ways commensurate with natural neighbour interpolation. If radix sort is used, then the computational complexity of the algorithm is linear with respect to input size. More specifically it is $O(\eta m d k)$ for d -dimensional data where each coordinate is represented using k bits and the combined total of query and data points is m . The number of iterations η is typically large but remains constant with increasing size of the data set. Hence it is likely that this approach will be useful in circumstances where interpolation is required for very large datasets. Note that η is likely to grow exponentially with respect to d , its precise relationship is left for future work.

The 1D interpolation schemes plugged in to the framework were selected for their simplicity and their amenability to further analysis. However more sophisticated methods could be used. For example basing the interpolation on 1D wavelets [5].

This framework can be extended to perform density estimation by simply replacing the interpolation function with a 1D density estimator. This is possible since the Hilbert curve has the property that it is *measure preserving*, which in the 2D case means that equal lengths along the curve correspond to equal areas. In this context the approach would fit in with the class of Monte Carlo density estimators such as random average shifted histograms [2].

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